ECE 656 Mini-Project
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Electrical engineers are familiar with the "semiconductor equations":

$$\nabla \bullet \vec{D} = \rho$$
$$\frac{\partial n}{\partial t} = -\nabla \bullet \left(\vec{J}_n / -q \right) + \left(G_n - R_n \right) \;, \tag{1}$$
$$\frac{\partial p}{\partial t} = -\nabla \bullet \left(\vec{J}_p / \; q \right) = \left(G_p - R_p \right)$$

which describe the flow of electrons and holes in semiconductors. These days, self-heating of electronic devices is a critical issue, so these equations need to be extended. We need to do two things. First, add a balance equation for heat (due to phonons **and** electrons) and modify the electron and hole currents to include the temperature dependence of the transport parameters and the effect of temperature gradients on current flow. **This assignment is about the balance equation for heat.** You may assume that we already have equations for the current flows.

From the BTE in the RTA, we derived the following equations:

$$\vec{J}_n = \sigma_n \vec{\nabla}\left(F_n / q \right) - S_n \sigma_n \vec{\nabla} T$$
$$\vec{J}_{Q_{el}} = \sigma_n T S_n \vec{\nabla}\left(F_n / q \right) - \kappa_0 \vec{\nabla} T \tag{2}$$
$$\vec{J}_{Q_{ph}} = -\kappa_{ph} \vec{\nabla} T$$

We can also express these equations in the inverted form as:

$$\vec{\nabla}\left(F_n / q \right) = \rho \vec{J}_n + S_n \vec{\nabla} T$$
$$\vec{J}_{Q_{el}} = T S_n \vec{J}_n - \kappa_n \vec{\nabla} T$$
$$\kappa_n = \kappa_0 - S_n^2 \sigma_n T \tag{3}$$
$$\vec{J}_{Q_{ph}} = -\kappa_{ph} \vec{\nabla} T$$

If you read papers and textbooks, you will find the heat balance equation written in different ways. The Domenicali equation is [1, 2]

$$c_{tot} \frac{\partial T}{\partial t} = \nabla \bullet \left(\kappa_{tot} \vec{\nabla} T \right) + \frac{\left| J_n^2 \right|}{\sigma_n} - T \frac{dS_n}{dT} \vec{\nabla} T \bullet \vec{J}_n \tag{4}$$

where c_{tot} is the total specific heat (electrons plus phonons) and κ_{tot} is the total thermal conductivity. Electronic device CAD tools often use the heat balance equation derived by Wachutka [3]

$$c_{tot}\frac{\partial T}{\partial t}=\nabla\bullet\left(\kappa_{tot}\vec{\nabla}T\right)+H \tag{5a}$$

$$H=\rho_n\left|J_n\right|^2-T\vec{\nabla}S_n\bullet\vec{J}_n-TS_n\nabla\bullet\vec{J}_n \tag{5b}$$

The objective of this project is to derive eqns. (4) and (5) and understand what approximations are involved in obtaining them.

This is a realistic problem of the type that you may expect to encounter more than once. For example, you may be using a simulation program to solve a problem. A careful user is always sure to understand what equations the simulation program is solving, where those equations came from, and what the underlying assumptions are.

You should approach this problem by beginning with our prescription for generating balance equations. This is a problem you should do on your own – do not discuss it with others. It is not as straightforward as a homework problem -- it will take some thought and trial and error. I can make a couple of suggestions to help you get started. You should begin by formulating a balance equation for the total heat (due to electrons and to phonons). As a first step, try to derive eqn. (30) of Wachutka [3]:

$$\begin{aligned}&c_{tot}\frac{\partial T}{\partial t}=\nabla\bullet\left(\kappa_{tot}\vec{\nabla}T\right)+H\\&H=\vec{J}_n\bullet\vec{\mathcal{E}}-\nabla\bullet\left(\pi\vec{J}_n\right)\end{aligned} \tag{6}$$

Then continue and try to get eqns. (5) and (4).

Your report will be due by 5:00 PM on the last day of class, Dec. 8, 2017. The report should explain how these equations can be derived from our balance equation approach and what assumptions are necessary to get these equations. The clarity of your report will be an important factor in grading. It should go without saying that all reports should be typewritten and nicely formatted.

[1] Charles A. Domenicali, "Irreversible Thermodynamics of Thermoelectricity," *Rev. Modern Phys.,* **26**, 237-235, 1954.

[2] Zhiting Tian, Sangyeop Lee, and Gang Chen, "A Comprehensive Review of Heat Transfer in Thermoelectric Materials," *Ann. Review of Heat Transfer,* **17**, 425-483, 2014.

[3] G.K. Wachutka, "Rigorous Thermodynamic Treatment of Heat Generation and Conduction in Semiconductor Device Modeling," *IEEE Trans. on Computer-Aided-Design*, **9**, 1141-1149, 1990.